



# Modeling of the Hydrocracking Reactor by the CESE Method

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## Abstract

In this article, the improved space-time conservation element and solution element (CESE) method are used to simulate the dynamic treatment of the hydrocracking reactor. The dynamic model consists of four lumps: vacuum gas oil (VGO), middle distillate, naphtha, and gas which is dissolved by this method. The offered method can solve the partial differential equations caused by the reactions inside the hydrocracking reactor. In this study, both temperature and mole fraction variables are solved explicitly and simultaneously. In the CESE method, to obtain a suitable answer to the dynamic model, a CFL insensitive scheme was used which, for the CESE method to be stable, the CFL number should be less than 1. In this work, obtained results from the CESE method, in good agreement with the data industry. Outcomes illustrate that AAD% of the yield forecast for the middle distillate, naphtha, and gas are 3.33%, 2.56 %, and 6.47%, respectively. This method unlike other contractual numerical methods treats with space and time coordinates Similar.

## Keywords:

CESE,  
Hydrocracking,  
Kinetic model,  
Modeling

## Introduction

The hydrocracking process is the most versatile of refinery conversion processes to promote heavy feedstocks to middle distillates. It can process a broad range of feedstocks from naphtha to asphalt to yield any favorable product with a molecular weight lower than that of the feedstock. The continuing advancements in this process are accredited to advancements in catalysts with ameliorate activity and selectivity, process adjustment, reactor plan, and access of relatively low-cost hydrogen from the amending process. Generally, Models are used to forecasts product yield and the effects of reactor operating conditions, such as pressure, temperature, and LHSV on the quality and yields of the products. Most researchers have worked on these lumping techniques and simulation of hydrocracking. In the writing, there are only a few released works on the numerical modeling of the hydrocracking process. Kumar and Sinha [1] reported a one-dimensional steady-state model to check the manner of hydrocracking reactions in the pivotal side of the reactor and examined the efficacy of various values of length of the reactor, temperature, and LHSV of the reactor on the product of yields. The ODEs characterizing the mass balances in the reactor were solved by the fourth-order Runge-Kutta method. Liu et. al [2] considered a dynamic model to simulation the hydrotreating process and investigated the efficacy of operating conditions such as bed temperature and LHSV on the reaction efficiency via simulate studies exerting the FDM. The method of CESE is a novel numeric method for dissolve equations of mass and energy hydrocracking reactor. It is the

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method proposed by Chang [3] from 1991 to the present. The CESE method has advantages: (1) it is an explicit scheme and differs the traditional numerical method [4], (2) High accuracy in capturing discontinuity, (3) good performance in non-reflecting boundary condition treatment. In the CESE method, both the autonomous current variables and their derivatives are behaved as unfamiliar and are dissolved at the same time. This reality that the CESE method is being with success applied to disciplines other than the ones that it emanated from, renders a powerful verification of the generality of this method. In the following, some of the works about the CESE method, which have appeared to date, are included. The CESE method was used to solve Euler and Navier-Stokes one-dimension equations in 1993 [5]. In 1995, Chang [4] Proposed a CESE method, and integrity explains the CESE method. In 1996, flows caused by shock-body interactions were studied using the CESE method [6]. Its application in unsteady flows with chemical reactions started in 1997. The propagation of voice waves via a nozzle by a shake wave was resolved using the CESE method in 2000 [7]. In 2019, this method was used for computational fluid dynamics [8] and in 2020, Checked out Numeric analysis of drops coagulation in fossa stream using the CESE method [9]. The goal is to solve the equations of mass and energy of the hydrocracking unit reactor.

## Reaction Network

This study considered four lumps, i.e., VGO, distillate, naphtha, and gas in accordance with the original products produced in a pilot-scale hydrocracking reactor. Fig. 1, illustrates the process pathways associated with the mentioned strategy.

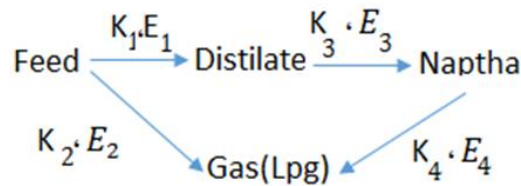


Fig. 1. Reaction scheme for kinetic model [10]

## Model Development

To develop the existing model, the under main suppositions are considered:

- Polymerization reaction and diffusion Effects are not in regard.
- Plug flow pattern in the hydrocracking reactor is assumed trickle-bed.
- Hydrogen feed is considered to be sheer.
- All the materials are considered in the liquid phase.
- Fixed catalyst activity has been considered.
- Hydrocracking reactions are considered first-order.

For each hydrocracking reactor reaction, a kinetic explanation ( $k$ ) is formulated as a subordinate of mole concentration and kinetic parameters ( $k_0, E$ ). Thus, the kinetic constants of the offered model are:

$$K_1 = K_{01} \exp\left(\frac{-E_1}{RT}\right) \quad (1)$$

$$K_2 = K_{02} \exp\left(\frac{-E_2}{RT}\right) \quad (2)$$

$$K_3 = K_{03} \exp\left(\frac{-E_3}{RT}\right) \quad (3)$$

$$K_4 = K_{04} \exp\left(\frac{-E_4}{RT}\right) \quad (4)$$

In Eqs. 1 to 4,  $R$  and  $T$  are the ideal gas constant and temperature, respectively. Therefore, the hydrocracking reaction ( $R_i$ ) is assumed:

$$\text{feed: } R_F = -k_1 C_F - k_2 C_F \quad (5)$$

$$\text{distillate: } R_D = k_1 C_F - k_3 C_D \quad (6)$$

$$\text{naphtha: } R_N = k_3 C_D - k_2 C_N \quad (7)$$

$$\text{gas: } R_G = k_1 C_F + k_4 C_N \quad (8)$$

where  $C_F$ ,  $C_D$ ,  $C_N$  and  $C_G$  are the mole concentration of VGO, distillate, naphtha, and gas. According to the law of conservation, mass and energy balances are written as follows:

$$\frac{dc_i}{dt} + \frac{d}{dv} (QC_i) = \epsilon J R_i \quad (9)$$

$$\frac{dT}{dt} + \frac{d(QT)}{dv} = \frac{\sum_{i=1}^m \epsilon J R_i (-\Delta H_r)}{\sum_{i=1}^n C_i C_{pi}} \quad (10)$$

where  $i$  is from VGO lump to gas;  $C$  is the mole concentration of lump;  $Q$  is the volume flow rate;  $\epsilon$  is the catalyst volume fraction (0.35) [10];  $J$  is the catalyst effectiveness factor (0.7) [10];  $C_{pi}$  is the heat capacity of component  $i$ ;  $\Delta H_r$  is the heat of the cracking reaction.

## Numerical Methods

### CESE Method

In the CESE method, flux conservation is executed both locally and globally over space and time. This flux conservation enforcement is an integral part of the process and no extrapolation or interpolation is needed. This method unlike other contractual numerical methods treats with space and time coordinates similar. For ease, Eqs. 9 and 10 can be rewritten in the under form:

$$\frac{dU_m}{dt} + \frac{dF_m}{dv} = R_m \quad (11)$$

where  $U_m = \begin{bmatrix} C_i \\ T \end{bmatrix}$ ,  $F_m = \begin{bmatrix} QC_i \\ QT \end{bmatrix}$  and  $R_m = \begin{bmatrix} \epsilon J R_i \\ \frac{\sum_{i=1}^m \epsilon J R_i (-\Delta H_r)}{\sum_{i=1}^n C_i C_{pi}} \end{bmatrix}$ . Let  $x_1 = v$  and  $x_2 = t$  denote the

coordinates of a Euclidean space  $E^2$ . By applying the Gaussian divergence theorem in  $E^2$ , Eq. 11 can be converted into the under integral protection form:

$$\oint_{sv} \vec{h}_m \cdot ds = \int_v R_m \quad (12)$$

where  $\vec{h}_m = (F_m, U_m)$  is the space-time flux in  $E^2$ , and  $S(V)$  is the border of a space-time region  $V$  in the  $E^2$ . Also, the right-hand side of Eq. 12 is a volume integration indicating the interior heat produced over region  $V$ .

As shown in Fig. 2, the Euclidean space  $E^2$  is segregated into an array of non-overlapping rectangular regions referred to as conservation elements (CEs). For any  $(v, t) \in SE(j, n)$ , let  $h_m$ ,  $F_m$  and  $U_m$  be approximated by  $h_m^*$ ,  $F_m^*$  and  $U_m^*$  respectively, can be demonstrated by the first-order Taylor series:

$$U_m^*(v, t; j, n) = U_m(n, j) + U_{mv}(n, j)(v - v_j) + U_{mt}(n, j)(t - t_j) \quad (13)$$

$$F_m^*(v, t; j, n) = F_m(n, j) + F_{mx}(n, j)(v - v_j) + F_{mt}(n, j)(t - t_j) \quad (14)$$

$$h_m^*(v, t; j, n) = (U_m^*(v, t; j, n), F_m^*(v, t; j, n)) \quad (15)$$

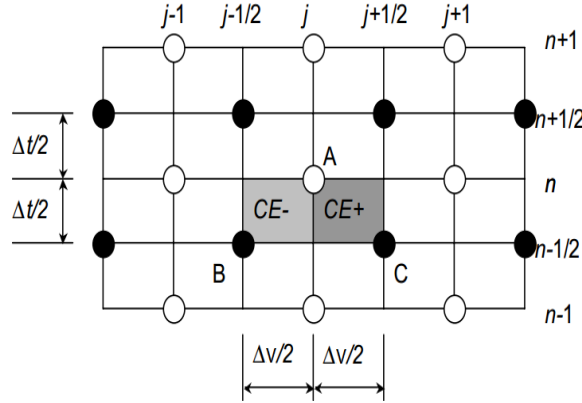


Fig. 2. Schematic image of CESE plot

Let for any \$(v, t) \in SE(j, n)\$, \$U\_m = U\_m^\*(v, t; j, n)\$ and \$F\_m = F\_m^\*(v, t; j, n)\$ in to Eq. 11:

$$\frac{\partial U_m^*(v, t; j, n)}{\partial t} + \frac{\partial F_m^*(v, t; j, n)}{\partial v} = R_m^* \quad (16)$$

The discrete approximation of Eq. 12 shows that:

$$\oint_{S(CE(j, n))} \vec{h}_m \cdot ds = (R_m)_j^n \times \frac{\Delta v \Delta t}{2} \quad (17)$$

Finally, by synthesizing Eqs. 11-17, it can be shown that:

$$\begin{aligned} U_m(n, j) - R_m(n, j) \times \frac{\Delta t}{2} \\ = \frac{1}{2} \left[ (U_m)_{j-\frac{1}{2}}^{n-\frac{1}{2}} + \frac{\Delta v}{4} (U_{mv})_{j-\frac{1}{2}}^{n-\frac{1}{2}} \right] + \frac{\Delta t}{2\Delta v} \left[ (F_m)_{j-\frac{1}{2}}^{n-\frac{1}{2}} + \frac{\Delta v}{4} (F_{mt})_{j-\frac{1}{2}}^{n-\frac{1}{2}} \right] \\ + \frac{1}{2} \left[ (U_m)_{j+\frac{1}{2}}^{n-\frac{1}{2}} - \frac{\Delta v}{4} (U_{mv})_{j+\frac{1}{2}}^{n-\frac{1}{2}} \right] - \frac{\Delta t}{2\Delta v} \left[ (F_m)_{j+\frac{1}{2}}^{n-\frac{1}{2}} + \frac{\Delta v}{4} (F_{mt})_{j+\frac{1}{2}}^{n-\frac{1}{2}} \right] \end{aligned} \quad (18)$$

Eq. 18 represents the input fluxes to point \$(n, j)\$ from points \$(n - \frac{1}{2}, j - \frac{1}{2})\$ and \$(n - \frac{1}{2}, j + \frac{1}{2})\$ for the numerical solution of \$U\_m(n, j)\$ from the previously computed values. \$(U\_{mv})\$ is given:

$$(u_{mv})_j^n = \frac{(u_m')_{j+\frac{1}{2}}^n - (u_m')_{j-\frac{1}{2}}^n}{\Delta v} + (2\varepsilon' - 1)(du_{mv})_j^n \quad (19)$$

Where \$\varepsilon'\$ is a parameter independent of numeric variables and its value is among 0 and 1 [11]. The CFL parameter controls the amount of the extended numeric dispersion. Here \$(u\_m')\_{j\pm\frac{1}{2}}^n\$ is

represented in the n-direction from point \$(u\_m)\_{j\pm\frac{1}{2}}^{n-\frac{1}{2}}\$, and thus the following form is obtained:

$$(u_m')_{j\pm\frac{1}{2}}^n \stackrel{\text{def}}{=} u_m_{j\pm\frac{1}{2}}^{n-\frac{1}{2}} + \frac{\Delta t}{2} (u_{mt})_{j\pm\frac{1}{2}}^{n-\frac{1}{2}} \quad (20)$$

$$(du_{mv})_j^n \stackrel{\text{def}}{=} \frac{(u_{mv})_{j+\frac{1}{2}}^{n-\frac{1}{2}} + (u_{mv})_{j-\frac{1}{2}}^{n-\frac{1}{2}}}{2} - \frac{u_m_{j+\frac{1}{2}}^{n-\frac{1}{2}} - u_m_{j-\frac{1}{2}}^{n-\frac{1}{2}}}{\Delta v} \quad (21)$$

By using the chain rule, for each  $m, k = F, D, N, G$  and  $T$  we have:

$$f_{mv} = \sum_{k=1}^m f_{m,k} \quad (22)$$

$$f_{mt} = \sum_{k=1}^m f_{m,k} u_{kt} \quad (23)$$

$$f_{m,k} = \frac{\partial f_m}{\partial u_k} \quad (24)$$

## Results and Discussion

Overall, Eqs. 11–24 show the usage of the CESE plot to the modeling of the coupled hydrocracking reactor. For simulation work, MATLAB software (Mathwork, Inc., 2013a) is used. By the CESE method and Eq. 18, both temperature and mole fraction (concentration) variables are solved explicitly and simultaneously. Fig. 3 shows the changes in temperature and mole fraction feed and product in unstable conditions. As shown in Fig. 3, over time feed becomes a valuable product in the hydrocracking reactor. Obviously, these conditions can create the maximum velocity of the volumetric flow within the specified range of operating conditions. ( $T=720^\circ K$ ,  $LHSV=1.05$ ,  $CFL < 1$ ). The kinetic parameters for each reaction are given in Table 1.

**Table 1.** Kinetic parameters for reactions

Activation energy	$kcal\ mol^{-1}$	Frequency factor	$m^3 h^{-1} m_{cat}^{-3}$
$E_1$	14.4	$K_{01}$	1.99E+05
$E_2$	10.11	$K_{02}$	2.29E+01
$E_3$	8.32	$K_{03}$	2.2E+02
$E_4$	6	$K_{04}$	133E-03

## Consistency Analysis

The consistency of the CESE method is investigated using the CFL number [12]. Such that if the under bet is limited, the answer is ever stable.

$$CFL \stackrel{\text{def}}{=} \frac{Q\Delta t}{\Delta v} \quad (25)$$

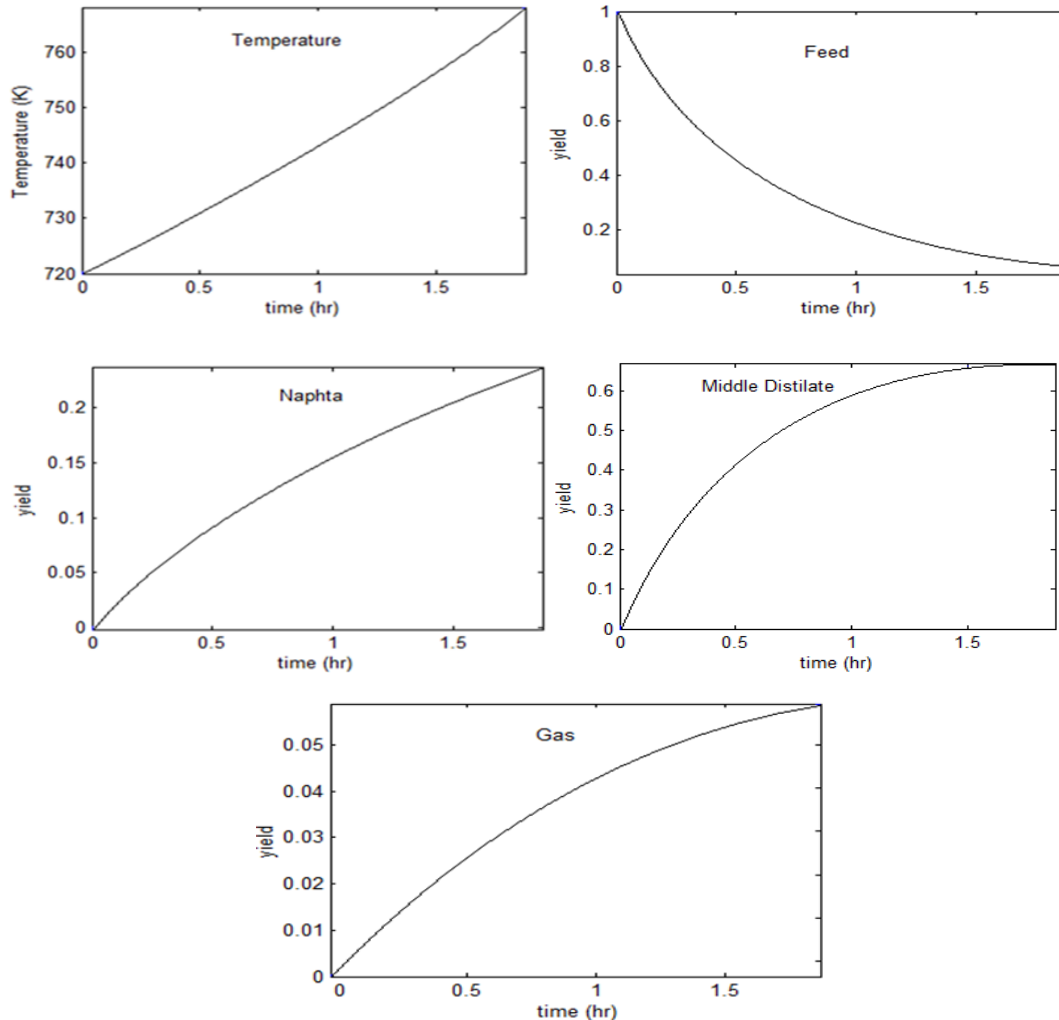
To calculate the number of CFL, the maximum rate is needed. This amount by Optimization using Genetic Algorithm is considered  $234.12\ m^3 hr^{-1}$ . The CESE parameters are determined as  $\Delta v = 0.95m^3$  and  $\Delta t = 0.00405hr$ , respectively. The results obtained are compared with the available plant data in Table 2 and Table 3.

**Table 2.** Comparison of simulated data using the CESE method and plant process data

	CESE method	plant data	AAD%
Distillate	0.6400	0.6620	3.33E-02
Naphtha	0.3622	0.2877	2.56E-01
Gas	0.0477	0.0510	6.47E-02

**Table 3.** Compare temperature simulated using the CESE method and plant process data

CESE method		plant data	
$T_{in}(K)$	$T_{out}(K)$	$T_{out}(K)$	AAD%
720	768.4	766	3.133E-03

**Fig. 3.** The response of the dynamic model dissolved by CESE ( $T=720^{\circ}K$ ,  $LHSV=1.05$ ,  $CFL < 1$ )

## Conclusions

The improved CESE method is used to simulate the dynamic treatment of the hydrocracking reactor. The dynamic model consists of four lumps: vacuum gas oil (VGO), middle distillate, naphtha, and gas which is solved by this method. The offered method can solve the partial differential equations resulting from the hydrocracking reactions. In this method, both temperature and mole fraction variables are solved explicitly and simultaneously. The CESE method could predict the yield of middle distillate, naphtha, gas, and temperature with AAD% of 3.33 %, 2.56%, 6.47%, and 3.13% respectively.

## Symbols used

AAD [%] absolute average deviation  
 CFL [-] courant Friedrichs levy

LHSV	[ $h^{-1}$ ]	liquid hourly space velocity
ODE	[-]	ordinary differential equation
S	[ $m^2$ ]	surface region
n	[-]	time step size Gas Reservoirs

### Abbreviations

BC	border condition
CE	conservation element
SE	solution element

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